

chain nodes :

1 2 3 4 5 6 7 8
26 27 33 34 42 43

chain bonds :

1-3 1-2 1-42 1-43 2-33 3-34 4-5 5-6 6-7 7-8 8-9 9-10 11-12 12-13 13-14 13-16
14-15 15-17 18-19 18-20 18-21 21-22 22-23 24-25 25-26 26-27

exact/norm bonds :

1-42 1-43 2-33 3-34
at hand

exact bonds :

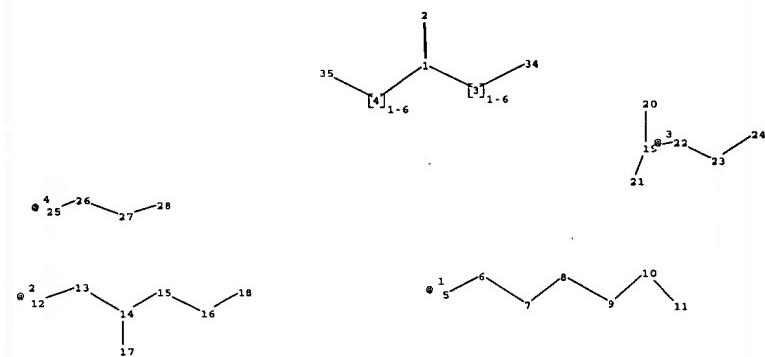
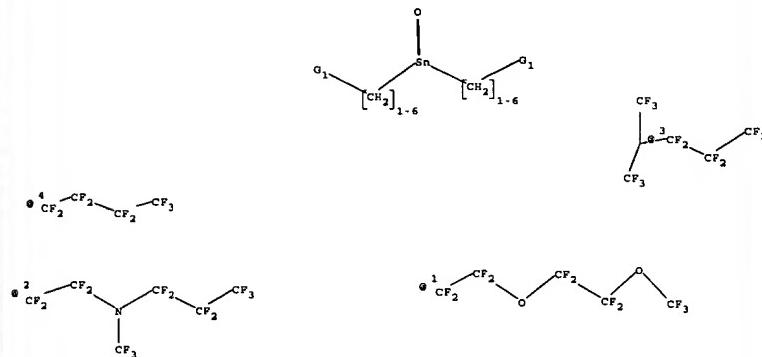
1-3 1-2 4-5 5-6 6-7 7-8 8-9 9-10 11-12 12-13 13-14 13-16 14-15 15-17 18-19
18-20 18-21 21-22 22-23 24-25 25-26 26-27

G1:CF3,[*1],[*2],[*3],[*4]

G2:X,Ak,Ph,OH,SH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,PhO,CN,NH2

Match Level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 33:CLASS
34:CLASS 42:CLASS 43:CLASS



chain nodes :

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
26	27	28	34	35																				

chain bonds :

1-2	1-3	1-4	3-34	4-35	5-6	6-7	7-8	8-9	9-10	10-11	12-13	13-14	14-15	14-17	
15-16	16-18	19-20	19-21	19-22	22-23	23-24	25-26	26-27	27-28						

exact/norm bonds :

3-34	4-35
------	------

exact bonds :

1-2	1-3	1-4	5-6	6-7	7-8	8-9	9-10	10-11	12-13	13-14	14-15	14-17	15-16	16-18	
19-20	19-21	19-22	22-23	23-24	25-26	26-27	27-28								

G1:CF3,[*1],[*2],[*3],[*4]

Match level :

1:CLASS	2:CLASS	3:CLASS	4:CLASS	5:CLASS	6:CLASS	7:CLASS	8:CLASS	9:CLASS	10:CLASS
11:CLASS	12:CLASS	13:CLASS	14:CLASS	15:CLASS	16:CLASS	17:CLASS	18:CLASS	19:CLASS	
20:CLASS	21:CLASS	22:CLASS	23:CLASS	24:CLASS	25:CLASS	26:CLASS	27:CLASS	28:CLASS	
34:CLASS	35:CLASS								

09/602,105

(FILE 'HOME' ENTERED AT 15:38:45 ON 29 SEP 2001)

FILE 'REGISTRY' ENTERED AT 15:39:00 ON 29 SEP 2001

L1 STRUCTURE uploaded
L2 QUE L1
L3 0 S L2
L4 0 S L2 FULL
L5 STRUCTURE uploaded
L6 QUE L5

=> d 15
L5 HAS NO ANSWERS
L5 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 16 full
FULL SEARCH INITIATED 15:43:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1220 TO ITERATE

100.0% PROCESSED 1220 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.04

L7 0 SEA SSS FUL L5

09/602,105

Trying 3106016892...Open

```
Welcome to STN International! Enter x:x  
LOGINID:sssptau124pxn  
PASSWORD:  
TERMINAL (ENTER 1, 2, 3, OR ?):2
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* * * * * * * * * * Welcome to STN International * * * * *

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| NEWS | 3 | Feb 06 Engineering Information Encompass files have new names |
| NEWS | 4 | Feb 16 TOXLINE no longer being updated |
| NEWS | 5 | Apr 23 Search Derwent WPINDEX by chemical structure |
| NEWS | 6 | Apr 23 PRE-1967 REFERENCES NOW SEARCHABLE IN CAPLUS AND CA |
| NEWS | 7 | May 07 DGENE Reload |
| NEWS | 8 | Jun 20 Published patent applications (A1) are now in USPATFULL |
| NEWS | 9 | JUL 13 New SDI alert frequency now available in Derwent's DWPI and DPCI |
| NEWS | 10 | Aug 23 In-process records and more frequent updates now in MEDLINE |
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| NEWS | 13 | Sep 17 IMSworld Pharmaceutical Company Directory name change to PHARMASEARCH |
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=>
Uploading C:\STNEXP4\QUERIES\602105.str

L1 STRUCTURE uploaded

=> que L1

L2 QUE L1

=> d his

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L1 STRUCTURE uploaded
L2 QUE L1

=> s 12 full

FULL SEARCH INITIATED 15:52:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1723 TO ITERATE

100.0% PROCESSED 1723 ITERATIONS
SEARCH TIME: 00.00.11

18 ANSWERS

L3 18 SEA SSS FUL L1

=> fil caplus

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SINCE FILE
ENTRY

TOTAL
SESSION
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134.33

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09/602,105

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=> s 13
L4 9 L3

=> d 1-9 bib abs

L4 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2001 ACS
AN 2001:27660 CAPLUS
DN 134:242980
TI Semi-Fluorinated Trialkyltin Fluorides and Fluorinated Telechelic Ionomers
as Viscosity-Enhancing Agents for Carbon Dioxide
AU Shi, Chunmei; Huang, Zhihua; Beckman, Eric J.; Enick, Robert M.; Kim, Sun-Young; Curran, Dennis P.
CS Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, 15261, USA
SO Ind. Eng. Chem. Res. (2001), 40(3), 908-913
CODEN: IECRED; ISSN: 0888-5885
PB American Chemical Society
DT Journal
LA English
AB Direct thickeners for dense carbon dioxide were designed and synthesized. Each thickener contained "CO₂-philic" fluorinated groups to impart solv. in carbon dioxide and "CO₂-phobic" functionalities to promote intermol. assocns. for viscosity enhancement. Semi-fluorinated trialkyltin fluorides and fluorinated telechelic ionomers were sol. to at least several wt. percent in dense liq. carbon dioxide without the use of a cosolvent. Increases in soln. viscosity at 297 K were measured using falling cylinder viscometry. The viscosity of liq. carbon dioxide was increased by a factor of 2-3 at thickener concns. of 2-4 wt. %. These results demonstrate that carbon dioxide viscosity enhancement is possible without the need for a cosolvent through the design of compds. with the appropriate balance of CO₂-philic groups for solv. and CO₂-phobic assocg. groups for macromol., viscosity-enhancing interactions. Neither compd., however, was as effective as the (29% styrene-71% fluoroacrylate) copolymer we recently developed. More substantial increases in soln. viscosity were not attained with the semi-fluorinated trialkyltin fluoride because the fluorinated alkyl chains disrupted the assocns. that formed viscosity-enhancing, weakly assocg., linear polymers. The viscosity

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increases obtained with the telechelic ionomer were also less than expected because of the relatively low mol. wt. of the carbon-dioxide-sol.

ionomers. Higher-mol.-wt. ionomers would not be CO₂-sol., however.

RE.CNT 29

RE

- (2) Cohen, L; US 3539311 1970 CAPLUS
- (3) Curran, D; J Am Chem Soc 1999, V121(28), P6607 CAPLUS
- (7) Enick, R; J Supercrit Fluids 1998, V13, P127 CAPLUS
- (8) Guan, Z; Macromolecules 1994, V27, P5527 CAPLUS
- (11) Harris, T; US 4913235 1990 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2001 ACS

AN 1999:410766 CAPLUS

DN 131:185032

TI Fluorous Tin Hydrides: A New Family of Reagents for Use and Reuse in Radical Reactions

AU Curran, Dennis P.; Hadida, Sabine; Kim, Sun-Young; Luo, Zhiyong

CS Department of Chemistry and Center for Combinatorial Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA

SO J. Am. Chem. Soc. (1999), 121(28), 6607-6615
CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

OS CASREACT 131:185032

AB Eight members of a new family of highly fluorinated (fluorous) tin hydrides have been synthesized and studied as reagents for radical reactions. Tin hydrides of the general formulas [Rf(CH₂)_n]₃SnH and [Rf(CH₂)_n]Me₂SnH (Rf = C₄F₉, C₆F₁₃, C₈F₁₇, C₁₀F₂₁; n = 2, 3) were prepd. These reagents are highly sol. in fluorinated solvents, and partition coeffs. between perfluorohexanes and several org. solvents have been measured. The reagents are generally useful for reductive radical reactions and hydrostannation reactions that would typically be conducted with tributyltin hydride. Stoichiometric and catalytic procedures have been developed, and both feature very easy seprn. of the tin products from the org. products by convenient liq.-liq. or solid-liq. extns. The tin reagents are recovered from reactions in high yields and are routinely reused. Rate const. measurements suggest that the fluorous tin hydrides are about as reactive as (or in some cases, slightly more reactive than) tributyltin hydride. The reagents show excellent potential for large-scale application in "green" (environmentally friendly) processes. In addn., they are useful for combinatorial and parallel synthesis applications both as reagents and as scavengers in phase-switching procedures.

RE.CNT 81

RE

- (2) Chatgilialoglu, C; Acc Chem Res 1992, V25, P188 CAPLUS
- (3) Chatgilialoglu, C; J Org Chem 1995, V60, P3826 CAPLUS
- (4) Clive, D; J Org Chem 1995, V60, P2607 CAPLUS
- (5) Cornils, B; Angew Chem Int Ed Engl 1997, V36, P2057 CAPLUS
- (6) Crich, D; J Org Chem 1996, V61, P7200 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2001 ACS

AN 1998:727787 CAPLUS

DN 130:66236

TI Rapid, parallel synthesis of homoallylic alcohols by Lewis acid mediated allylations of aldehydes with new fluorous allyl stannanes

AU Curran, Dennis P.; Luo, Zhiyong

09/602,105

CS Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260,
USA
SO Med. Chem. Res. (1998), 8(4/5), 261-265
CODEN: MCREEB; ISSN: 1054-2523
PB Birkhaeuser Boston
DT Journal
LA English
AB Parallel Lewis acid mediated allylations of four arylaldehydes with two fluorous allylstannanes are reported. These stannanes tris-(4,4,5,5,6,6,7,7,8,8,9,9-tridecafluororononyl)allylstannane and tris-(4,4,5,5,6,6,7,7,7-nonafluoroheptyl)allylstannane bear propylene spacers between the fluoroalkyl groups and the Sn and seem to behave like normal trialkylstannanes in SnCl_4 promoted allylations. Reactions are purified by quenching with base and filtration through fluorous reverse phase silica gel. The procedure is prototypical of a general method to use fluorous reagents for conducting ionic reactions in parallel.

RE.CNT 21

RE

- (1) Cornils, B; Angew Chem Int Ed 1997, V36, P2057 CAPLUS
(4) Curran, D; Chemtracts-Org Chem 1996, V9, P75 CAPLUS
(5) Curran, D; J Am Chem Soc 1996, V118, P2531 CAPLUS
(6) Curran, D; J Org Chem 1996, V61, P6480 CAPLUS
(7) Curran, D; J Org Chem 1997, V62, P6714 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2001 ACS

AN 1998:630478 CAPLUS

DN 129:330310

TI "Propylene spaced" allyl tin reagents: a new class of fluorous tin reagents for allylations under radical and metal-catalyzed conditions

AU Curran, Dennis P.; Luo, Zhiyong; Degenkolb, Peter

CS Department Chemistry, University Pittsburgh, Pittsburgh, PA, 15260, USA

SO Bioorg. Med. Chem. Lett. (1998), 8(17), 2403-2408

CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

AB A new generation of propylene-spaced fluorous allyltin reagents $[(\text{Rf}(\text{CH}_2)_3)_3\text{SnCH}_2\text{CH}=\text{CH}_2]$ [$\text{Rf} = \text{CF}_3(\text{CF}_2)_n(\text{CH}_2)_3$; $n = 5, 3$] is described. These succeed in radical allylations where their lower homologs (ethylene-spaced) fail, and they provide improved performance in transition metal catalyzed allylations. The reagents and byproducts are readily sepd. by simple fluorous-org. liq.-liq. or solid-liq. extns.

L4 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2001 ACS

AN 1983:595223 CAPLUS

DN 99:195223

TI Tris-(γ -trifluoropropyl)chlorostannane

IN Mironov, V. F.; Yankov, V. V.; Stepina, E. M.; Kuptsova, T. S.; Shiryaev, V. I.

PA USSR

SO U.S.S.R.

From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1983, (24), 206.

CODEN: URXXAF

DT Patent

LA Russian

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|------------|------|----------|-----------------|----------|
| PI | SU 536680 | A1 | 19830630 | SU 1975-2137216 | 19750526 |

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AB $(F_3CCH_2CH_2)_3SnCl$ was prep'd. by treating $F_3CCH_2CH_2Cl$ with Sn (3-10:1 molar ratio) at 100-200.degree. in the presence of amine or phosphine catalyst (0.1-0.5 mol/mol Sn) and iodine or iodine-contg. compd. cocatalyst (0.05-0.2 mol/mol Sn).

L4 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2001 ACS

AN 1978:509698 CAPLUS

DN 89:109698

TI Direct preparation of organotin biocides

AU Stepina, E. M.; Yankov, V. V.; Gulo, R. A.; Kuptsova, T. S.; Mironov, V. F.

CS Minist. Khim. Prom., Moscow, USSR

SO Biol. Akt. Soedin. Elemt. IV B Gruppy (1977), 231-4 Publisher: Akad. Nauk SSSR, Sib. Otd., Irkutsk. Inst. Org. Khim., Irkutsk, USSR.

CODEN: 38OBA2

DT Conference

LA Russian

AB $(F_3CCH_2CH_2)_3SnCl$ was prep'd. in 80% yields by heating $F_3CCH_2CH_2Cl$ with Sn in presence of amines and iodine at 170-80.degree.. Test data for its antiseptic properties were given.

L4 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2001 ACS

AN 1971:488765 CAPLUS

DN 75:88765

TI Fluoroalkyltin compounds

IN Murch, Robert M.

PA Dow Corning Corp.

SO U.S., 2 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------|----------|-----------------|----------|
| PI | US 3590060 | A | 19710629 | US 1969-860028 | 19690922 |
| AB | 3,3,3-Trifluoropropyltin compds. are prep'd. for use as stabilizers in polyvinyl resins, catalysts, pesticides, bactericides, and oil repellents. | | | | |
| | CF ₃ (CH ₂) ₂ MgBr was treated with SnCl ₄ to give tetrakis(3,3,3 - trifluoropropyl)tin. (3,3,3 - Trifluoropropyl)triphenyltin and tris(3,3,3-trifluoropropyl)methoxytin were among 9 compds. similarly prep'd. | | | | |

L4 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2001 ACS

AN 1970:409206 CAPLUS

DN 73:9206

TI Nuclear magnetic resonance coupling constants in tin in 3,3,3-trifluoropropyltin compounds

AU Williams, Dwight Edward; Toporcer, Louis H.; Ronk, Gary M.

CS Dow Corning Corp., Midland, Mich., USA

SO J. Phys. Chem. (1970), 74(10), 2139-42

CODEN: JPCHAX

DT Journal

LA English

AB The various NMR coupling consts. between Sn and H and F have been detd. from the heteronuclearly decoupled ¹H and ¹⁹F NMR spectra of eleven 3,3,3-trifluoropropyltin compds. These results are discussed in the light

of the Barfield alternate MO theory of spin coupling. The invalidity of the use of coupling consts. to det. hybridization is briefly discussed. For these data it was not necessary to invoke a "spatial mechanism" of

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spin coupling. The vicinal Sn-H coupling const. was larger than the geminal Sn-H coupling const. in most instances despite reports that the opposite case is a characteristic of metal-alkyl compds. These data indicate that a postulated intramol. interaction between Sn and F does not occur.

L4 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2001 ACS
AN 1970:72974 CAPLUS
DN 72:72974
TI Orbital populations and .pi. backbonding in some organohalostannanes: interpretation of tin Moessbauer and ligand NQR[nuclear quadrupole resonance] data
AU Williams, Dwight Edward; Kocher, C. W.
CS Dow Corning Corp., Midland, Mich., USA
SO J. Chem. Phys. (1970), 52(3), 1480-8
CODEN: JCPSA6
DT Journal
LA English
AB Tin Moessbauer isomer shifts and quadrupole splittings are reported for
23 compds. Equations are derived and applied which enable the Sn hybrid orbital populations for tetravalent Sn compds. of the type $AmSnB4-m$ to be detd. from the above data. Crit. tests of the theory are proposed. A min. value of 5.8 mm sec⁻¹ is obtained for the quadrupole splitting due to one p electron by comparing Moessbauer-derived with ligand NQR-derived populations. The two sets of populations are also used to obtain .pi. backbonding orbital populations in organohalostannanes. The Sn sp³ orbitals are more important than d orbitals for .pi. back-bonding.